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Universality check of the overlap fermions in the Schrödinger functional

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I examine some properties of the overlap operator in the Schroedinger functional formulated by Lüscher at perturbative level. By investigating spectra of the free operator and one-loop coefficient of the Schroedinger functional coupling, I confirm the universality at tree and one-loop level. Furthermore, I address cutoff effects of the step scaling function and it turns out that the lattice artifacts for the overlap operator are comparable with those of the clover actions.

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1. Introduction

As well known, the overlap fermions [1] have an exact chiral symmetry on the lattice, that is, the fermion operator satisfies the Ginsberg-Wilson (GW) relation. This is an ideal formulation to compute the quark condensate, which is an important physical quantity as an order parameter of the spontaneous symmetry breaking, without running into the subtle additive renormalization problem. A renormalized quark condensate depends on the renormalization scale and scheme, but, in order to avoid such dependences it is usually convenient to choose a renormalization group invariant (RGI) as a reference quantity,

$$\Sigma_{\text{RGI}} = \lim_{g_0 \to 0} \mathscr{Z}_{\text{P}}(g_0) \Sigma_{\text{lat}}(g_0), \tag{1.1}$$

where I have used the fact that thanks to the chiral symmetry on the lattice the renormalization factors for the flavor singlet scalar and the flavor non-singlet pseudo-scalar density are equivalent even at a finite lattice spacing. Recently, the JLQCD collaboration [2] estimated the bare quark condensate, and then performed the renormalization through a non-perturbative scheme, so called, RI/MOM scheme. However, in order to carry out the renormalization in a solid way, here I will use more sophisticated scheme, the Schrödinger functional (SF) scheme. As well known this scheme can be defined non-perturbatively at massless point, and can avoid the large scale problem.

Now let me explain how to carry out the non-perturbative renormalization of the quark condensate by making use of the SF scheme. My final goal is the RGI condensate in eq.(1.1). In order to get this quantity from the given bare quantity the renormalization factor $\mathscr{Z}_{\text{P}}(g_0)$ is required. This factor can be obtained by the following renormalization program which is divided into three parts.

$$\mathscr{Z}_{\text{P}}(g_0) = \hat{Z}_{\text{P,SF}}^{\text{PT}}(\infty, \mu_{\text{PT}}) U_{\text{P,SF}}^{\text{NP}}(\mu_{\text{PT}}, \mu_{\text{had}}) Z_{\text{P,SF,ov}}^{\text{NP}}(g_0, a\mu_{\text{had}}). \tag{1.2}$$

First, the left factor $\hat{Z}_{\text{P,SF}}^{\text{PT}}(\infty, \mu_{\text{PT}})$ is required to remove the scale and scheme dependence of the quark condensate. If the energy scale μ_{PT} is so high then it is sufficient to use perturbation theory to get this factor. The middle factor represents the non-perturbative evolution of Z_{P} from a low energy μ_{had} to the high energy scale. Actually a product of this factor and the previous one was already calculated by the ALPHA collaboration [3] for $N_{\text{f}} = 2$ in the SF scheme. Note that it is independent of the discretization, that is, the lattice action. The right factor, $Z_{\text{P,SF,ov}}^{\text{NP}}(g_0, a\mu_{\text{had}})$, is a renormalization factor relating the bare quark condensate and a renormalized one at a certain renormalization scale, which should be low energy μ_{had} in order to avoid large cutoff effects. In fact, the last factor is a missing piece to get the RGI. Since this factor depends not only on the scale and the scheme but also the lattice action (now it is the overlap fermion), first of all, one has to define the overlap fermion in the SF.

In the next section, I will briefly introduce the formulation proposed by Lüscher. I will not compute Z_{P} in this report, instead I will show some preparative studies, spectra of free operator and universality check at both tree and quantum level. Furthermore I will address cutoff effects for the overlap fermion at one-loop level. More details about results shown in the report can be found in Ref. [4].

2. Formulations of the overlap fermion in SF

Since the boundary conditions of the SF are not compatible with the chiral symmetry, it is

not so trivial to formulate the overlap fermions in the SF. An important issue is how to break the GW relation while keeping the boundary conditions (up to $O(a)$). So far, three formulations have been proposed. First one is an orbifolding construction by Taniguchi [5], which contains some subtleties. However, as Sint showed in Ref. [6], such subtleties can be partially removed by introducing a chirally rotated version of the SF. Nevertheless, this is rather technically involved. In this report, I take rather simpler one, so called universality formulation proposed by Lüscher [7].

Let me introduce the universality formulation briefly. A massless operator is given by

$$\bar{a}D_{\mathrm{N}} = 1 - \frac{1}{2}(U + \gamma_5 U^\dagger \gamma_5), \qquad \bar{a} = a/(1+s), \tag{2.1}$$

$$U = AX^{-1/2}, \qquad X = A^\dagger A + caP, \qquad A = 1 + s - aD_{\mathrm{w}}, \tag{2.2}$$

where s is a tunable parameter to optimize computational costs, and D_{w} is the Wilson operator in the SF. A crucial difference of the overlap operator in the usual lattice and that in the SF is the presence of an operator P in the inverse square root. This operator is supported near boundary and plays an important role to produce the correct boundary conditions in the continuum limit. Due to the presence of P, the matrix U is not unitary anymore. Accordingly the overlap operator does not satisfy the GW relation, instead it follows the modified relation,

$$\gamma_5 D_{\mathrm{N}} + D_{\mathrm{N}}\gamma_5 = \bar{a}D_{\mathrm{N}}\gamma_5 D_{\mathrm{N}} + \Delta_B, \tag{2.3}$$

with a breaking term Δ_B. It is shown [7] that this breaking term is exponentially suppressed away from the boundary, therefore, the chiral symmetry is approximately maintained in the bulk. The coefficient c in eq.(2.2) has an important role to cancel $O(a)$ corrections of physical quantities, and it has a perturbative expansion

$$c = c^{(0)} + g_0^2 c^{(1)} + O(g_0^4). \tag{2.4}$$

According to the original paper, I set the tree value $c^{(0)} = 1 + s$, which is an optimal choice for the tree level O(a) improvement, in the following calculations.

In the definition of the overlap operator, there is the inverse square root. Due to the presence of the background field, the kernel of the inverse square root is not diagonal matrix anymore even in the free case and even after performing partial Fourier transformations. Therefore I have to rely on the numerical approximation even in the perturbative calculation. To this end, I use the minimax polynomial approximation [8],

$$X_{\mathbf{p}}^{-1/2} \approx \sum_{k=0}^{N} c_k T_k((2X_{\mathbf{p}} - v_{\mathbf{p}} - u_{\mathbf{p}})/(v_{\mathbf{p}} - u_{\mathbf{p}})), \tag{2.5}$$

where T_k is the Chebyshev polynomial of degree k. $X_{\mathbf{p}}$ is a kernel in the time-momentum space whose size is $4(T/a - 1)$ square for a fixed spatial momentum configuration $\mathbf{p}$, and the minimal and maximum eigenvalues of $X_{\mathbf{p}}$ are denoted by $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ respectively. The coefficient c_k is determined by the Remez algorithm to obtain the Minimax polynomial. In the summation step, I use the Clenshaw sum scheme in order to maintain numerical precisions. An accuracy for the approximation is set to 10^{-13}. Given this accuracy, a ratio between the minimum and maximum eigenvalue determine the degree of polynomial. In my computation, $u_{\mathbf{p}}/v_{\mathbf{p}} \sim 0.01$ for a typical case. Then the degree of polynomial turns out to be $N \sim 100$. This is just for a purpose to give some feeling.
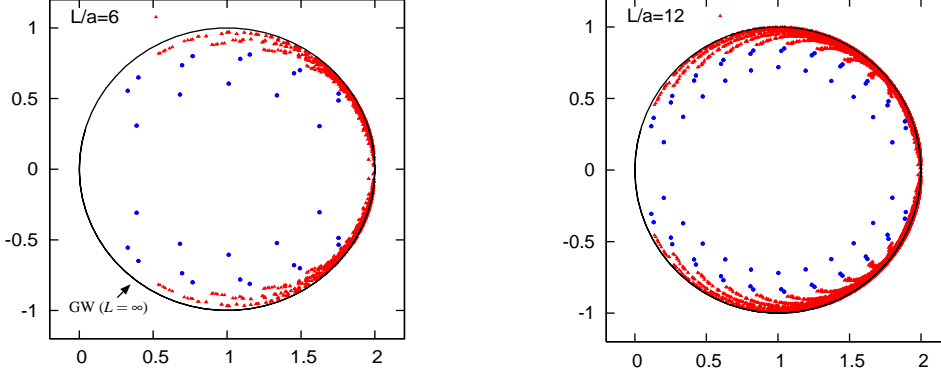
Figure 1: Spectrum of $\bar{a}D_N$ with $s = 0$ and $\theta = 0$ in the presence of the background field.

3. Spectrum of free operator

Spectra of the free massless operator $\bar{a}D_N$ are shown in Figure 1 for $L/a = 6, 12$. The parameters are set to $s = \theta = 0$ where θ parameterizes the generalized boundary conditions for the spatial directions. The non-vanishing background gauge field [9] is used here. Blue points, which belong to a zero spacial momentum sector, and red points, which are from the other sector, represent individual eigenvalues. Actually in the original paper [7], it is shown that the operator is bounded by a unit circle

$$||\bar{a}D_N - 1|| \leq 1, \tag{3.1}$$

and it is given by the black solid circle in the plot. This equation indicates that all eigenvalues are contained in the circle. On the other hand, in the infinite volume case, that is, the usual GW fermion, it is known that all eigenvalues lie on the circle. Therefore the deviation from the circle is considered as boundary effects or finite size effects and actually such deviation is reduced for larger lattice in the right panel of Figure 1. Especially I found that the blue points are strongly affected by the boundary effects in the sense that they are distant from the circle.

Furthermore, I investigate spectra of hermitian operator $L^2 D_N^\dagger D_N$. Actually the eigenvalues for this operator have continuum limit [10]. Figure 2 shows scaling behaviors of the ten lowest eigenvalues. All cases converge to the continuum limit properly for both θ values. Therefore I conclude that the universality at the tree level is confirmed.

4. Universality check in perturbation theory

In the previous section I have investigated the property of the free operator. In this section, let me address the universality at the quantum level. For the purpose, I consider the SF coupling [9, 10]

$$\bar{g}_{SF}^2(L) = \left. \frac{\partial \Gamma}{\partial \eta} \right|_{\eta = v = 0} = g_0^2 [1 + m_1(L/a)g_0^2 + O(g_0^4)], \tag{4.1}$$

where Γ is an effective action of the system and the standard convention $T = L$ is taken. Now I am interested in the one-loop contribution $m_1(L/a)$. This is composed from the gauge and fermion
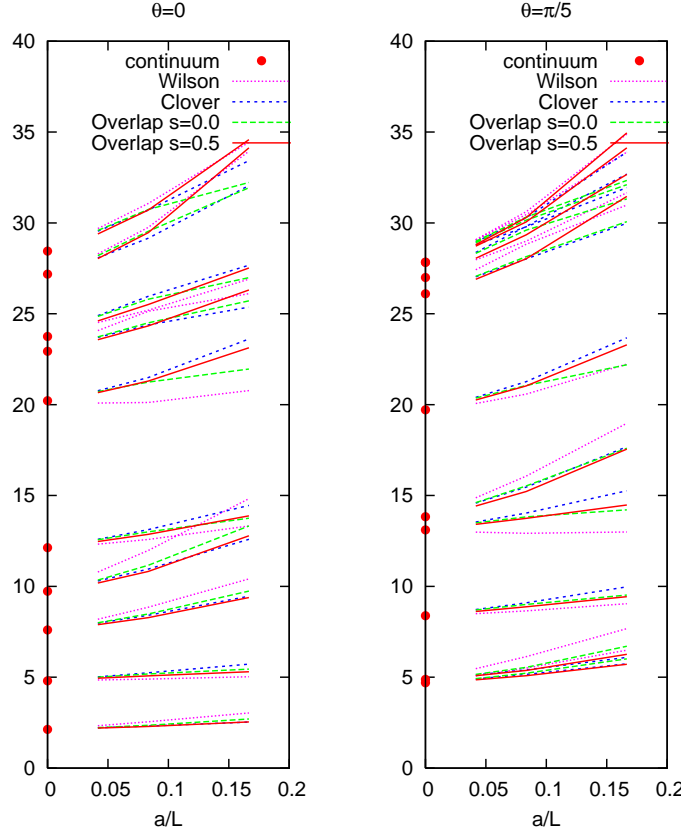
Figure 2: Spectrum of $L^2 D_N^\dagger D_N$ with $\theta = 0$ (left) and $\theta = \pi/5$ (right) in the presence of the background field. The red points represent the continuum values from [10].

parts, $m_1(L/a) = m_{1,0}(L/a) + N_f m_{1,1}(L/a)$, and I compute the fermion part numerically by using the overlap operator. And then I analyze the data according to the Symanzik's expansion form

$$m_{1,1}(L/a) = A_0 + B_0 \ln(L/a) + A_1 a/L + B_1 a/L \ln(L/a) + O((a/L)^2). \tag{4.2}$$

I extract first few coefficients, A_0, B_0,... by making use of the method in Ref. [11].

The first coefficient A_0 is generally a function of the parameter s, and I get $A_0(s)|_{s=0} = 0.012567(3)$, while by combining the results of Ref. [10, 12], $A_0(s)|_{s=0} = 0.012566$ can be deduced. Consistency can be seen with a reasonable degree of accuracy. B_0 is a coefficient of the log divergence and this is related with the fermion part of the one-loop coefficient of the beta function, $b_0^F = -1/(24\pi^2)$. I confirm $B_0 = 2b_0^F$ up to 4 digits for several values of s. From these results, I can conclude that the universality at the quantum level is confirmed. Furthermore, I determined A_1 as a function of s. Actually this gives fermion part of the $O(a)$ boundary counter term at one-loop order, $c_t^{(1)} = c_t^{(1,0)} + N_f c_t^{(1,1)}$,

$$c_t^{(1,1)} = A_1/2 = -0.00958 - 0.00206s - 0.00484s^2 - 0.00748s^3 - 0.01730s^4. \tag{4.3}$$

This formula will be used for future simulations to achieve one-loop $O(a)$ improvement. I checked
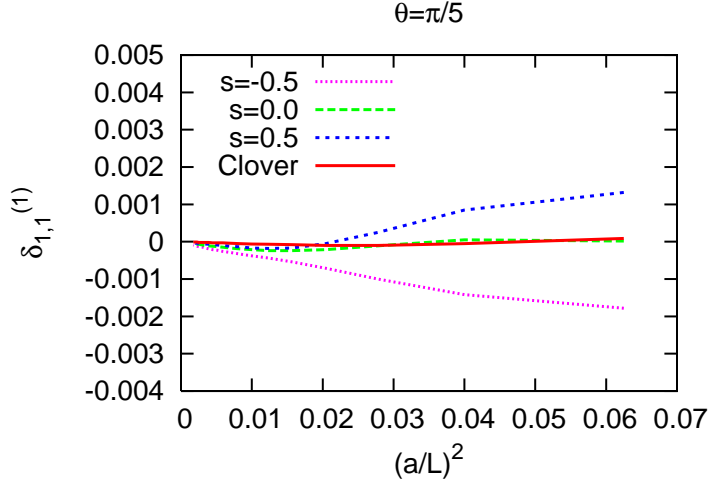
Figure 3: One-loop relative deviation as a function of $(a/L)^2$ with $\theta = \pi/5$.

$B_1 = 0$ up to few digits. Since this is a signal for tree level O(a) improvement, I can confirm this in an actual manner.

5. Lattice artifacts of step scaling function

Finally let me show lattice artifacts of the step scaling function, which describes the evolution of the running coupling,

$$\sigma(u) = \bar{g}^2(2L), \qquad u = \bar{g}^2(L). \tag{5.1}$$

The relative deviation is defined as

$$\delta(u, a/L) = \frac{\Sigma(u, a/L) - \sigma(u)}{\sigma(u)} = \delta_1(a/L)u + O(u^2), \tag{5.2}$$

where $\sigma(u)$ represents the step scaling function in the continuum limit and $\Sigma(u, a/L)$ is that on the lattice, and this tells us the size of lattice artifacts. I evaluate the fermion part of this quantity to one-loop order, $\delta_1(a/L) = \delta_{1,0}(a/L) + N_\mathrm{f}\delta_{1,1}(a/L)$.

Figure 3 shows its scaling behavior. Note that the overlap fermion with $s = 0$ shows almost flat, and this value of s is an optimal choice from the point of view of lattice artifacts. For comparison, I include the results of the clover action [10], and it also shows small cutoff effects. Therefore I conclude that the lattice artifacts of the clover and the overlap fermion with $s = 0$ are comparable.

6. Concluding remarks

Among some formulations, I choose Lüscher's formulation. I investigate the spectra of the free overlap operators, and then I observe the expected behaviors. Next, I confirm the universality at quantum level, and determine the O(a) boundary counter term at one-loop order, $c_\mathrm{t}^{(1,1)}$. This is needed in future simulations to reduce cutoff effects. Furthermore I investigate the lattice artifacts

of the step scaling function to one-loop order, and then it turns out that the scaling behavior of the overlap is comparable with the clover action.

As next targets, there are several quantities within perturbation theory. In this report, I exclusively consider the massless case, however, I will investigate massive case too. A comparison study with the orbifolding formulations is also interesting. Furthermore, still there is an improvement coefficient which I have to compute before starting simulations, $c^{(1)}$ in eq.(2.4). In fact the coefficients c is only accessible within a framework of perturbation theory, therefore two-loop calculations will be required. In that course, it is very convenient to use the automatic method developed last year [13].

Finally, I have to remind readers that my final goal is the non-perturbative computation of Z_P.

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